

On the thermodynamic stability conditions of Tsallis' entropy

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Abstract

The thermodynamic stability condition (TSC) of Tsallis' entropy is revisited. As Ramshaw [Phys. Lett. A **198** (1995) 119] has already pointed out, the concavity of Tsallis' entropy with respect to the internal energy is not sufficient to guarantee thermodynamic stability for all values of q due to the non-additivity of Tsallis' entropy. Taking account of the non-additivity the differential form of the TSC for Tsallis entropy is explicitly derived. It is shown that the resultant TSC for Tsallis' entropy is equivalent to the positivity of the standard specific heat. These results are consistent with the relation between Tsallis and Rényi entropies.

Key words: Thermodynamic stability, Tsallis' entropy, Pseudo-additivity

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Since the pioneering work of Tsallis in 1988 [1] there has been growing interest in the nonextensive thermostatistics [2] based on Tsallis' entropy defined by

$$S_q^T = \frac{1 - \sum_i p_i^q}{q - 1}, \quad (1)$$

where p_i is a probability that a system of interest in state i , and q is a real parameter. For the simplicity the Boltzmann constant sets to unity throughout this paper. The nonextensive thermostatistics is a generalization of the standard Boltzmann-Gibbs (BG) statistical mechanics by the real parameter q . In the $q \rightarrow 1$ limit, S_q^T reduces to BG entropy $S_1^T = -\sum_i p_i \ln p_i$. One of the most distinct properties of Tsallis' entropy is the *pseudo-additivity*:

$$S_q^T(A, B) = S_q^T(A) + S_q^T(B) + (1 - q)S_q^T(A)S_q^T(B), \quad (2)$$

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where A and B are two subsystems in the sense that the probabilities of the composed system $A + B$ factorize into those of A and of B . The entropic index q characterizes the degree of non-extensivity of the system through the pseudo-additivity.

It is shown that some important thermodynamical properties, such as the Legendre structure [3–5], hold true for the nonextensive thermostatistics. The thermodynamic stability plays an important role in any formalism related to thermodynamics. The conventional thermodynamic stability arguments [6] are based on the extremum principle and the additivity of entropy, whereas the nonextensive thermostatistics is based on the non-additive entropy S_q^T . Therefore the thermodynamic stability in the nonextensive thermostatistics is one of the most important and nontrivial properties. For the earlier versions of the nonextensive thermostatistics [1,3], Ramshaw [7] had first indicated that the concavity of S_q^T is not sufficient to guarantee thermodynamic stability of the nonextensive Tsallis entropy S_q^T for all values of q . Next Tsallis [8] had shown that if we use the un-normalized internal energy $U_{q,\text{un}} \equiv \sum_i p_i^q \epsilon_i$, instead of standard one $U \equiv \sum_i p_i \epsilon_i$, the concavity (or convexity) of S_q^T with respect to $U_{q,\text{un}}$, i.e., $q(\partial^2 S_q^T / \partial U_{q,\text{un}}^2) \leq 0$, is recovered. He thus concluded that the thermodynamic stability for all q is rescued if $U_{q,\text{un}}$ is used. For the latest version [2,4] of nonextensive thermostatistics, in which the normalized internal energy $U_q \equiv \sum_i p_i^q \epsilon_i / \sum_j p_j^q$ is used, de Silva *et al.* [9] shown that C/q is nonnegative for $q \notin [0, 1]$, where C stands for the specific heat defined by $C \equiv \partial U_q / \partial T$ and T is the temperature. Lenzi *et al.* [10] have shown the specific heat C is positive for all values of q when the normalized Tsallis' entropy [11] defined by $S_{q,\text{no}}^T \equiv S_q^T / \sum_i p_i^q$, is used instead of S_q^T

However, what they have shown are the concavity (or convexity) of Tsallis' entropy with respect to the appropriate internal energy or the positivity (or negativity) of the specific heat. As Ramshaw has originally pointed out, the concavity of S_q^T with respect to internal energy is not sufficient to guarantee the thermodynamic stability of nonextensive systems described by S_q^T , since the conventional thermodynamic stability arguments [6] are based on the additivity of entropy and since S_q^T is not additive. The essence of thermodynamic stabilities lies in the entropy maximum principle [6]. For an additive entropy $S(U)$, e.g., Boltzmann–Gibbs or Rényi one, the relation between the concavity of $S(U)$ and thermodynamic stability is straightforward as follows. If we were remove an amount of energy ΔU from one of two identical subsystems and transfer it to the other subsystem, the total entropy would change from its initial value of $2S(U)$ to $S(U + \Delta U) + S(U - \Delta U)$. The entropy maximum principle demands that the resultant entropy is not larger than the initial entropy, i.e.,

$$2S(U) \geq S(U + \Delta U) + S(U - \Delta U), \quad (3)$$

which is the TSC for the additive entropy $S(U)$. In the limit of $\Delta U \rightarrow 0$, Eq. (3) reduces to its differential form

$$\frac{\partial^2 S(U)}{\partial U^2} \leq 0, \quad (4)$$

which states the concavity of $S(U)$. Thus the TSC and the concavity of $S(U)$ with respect to U are equivalent each other when $S(U)$ is additive. However this is not the case for the non-additive entropy S_q^T . In this letter the TSC for the non-additive Tsallis' entropy S_q^T is reconsidered.

Let us begin by deriving the differential form of the TSC for S_q^T . Taking account of the pseudo-additivity of Eq. (2), the TSC for S_q^T can be written by

$$2S_q^T(E) + (1-q) \left[S_q^T(E) \right]^2 \geq S_q^T(E + \Delta E) + S_q^T(E - \Delta E) + (1-q)S_q^T(E + \Delta E)S_q^T(E - \Delta E), \quad (5)$$

where E stands for an additive internal energy, e.g., U or U_q . The physical meaning of this inequality is same as that of the conventional TSC Eq. (3). If we were remove an amount of energy ΔE from one of two identical subsystems and transfer it to the other subsystem, the total entropy would change from its initial value of the right-hand-side to the left-hand-side of Eq. (5). The entropy maximum principle demands that the resultant entropy is not larger than the initial entropy. The difference between Eqs. (5) and (3) is the presence of the nonlinear terms proportional to $1 - q$, which originally arise from the pseudo-additivity of S_q^T .

For $\Delta E \rightarrow 0$, Eq. (5) reduces to its differential form:

$$\frac{\partial^2 S_q^T(E)}{\partial E^2} + (1-q) \left\{ S_q^T(E) \frac{\partial^2 S_q^T(E)}{\partial E^2} - \left(\frac{\partial S_q^T(E)}{\partial E} \right)^2 \right\} \leq 0, \quad (6)$$

Introducing the generalized temperature T_q ,

$$\frac{1}{T_q} \equiv \frac{\partial S_q^T}{\partial E}, \quad (7)$$

and generalized specific heat C_q ,

$$\frac{1}{C_q} \equiv \frac{\partial T_q}{\partial E} = -T_q^2 \frac{\partial^2 S_q^T}{\partial E^2}, \quad (8)$$

Eq. (6) reduces to

$$\frac{1 + (1 - q)S_q^T}{C_q} + (1 - q) \geq 0, \quad (9)$$

or by utilizing the definition Eq. (1) of S_q^T and the relation $\sum_i p_i^q = Z_q^{1-q}$ [2,4], Eq. (9) can be cast into the form,

$$\frac{Z_q^{1-q}}{C_q} + (1 - q) \geq 0, \quad (10)$$

where Z_q is the generalized partition function. In this way the positivity of C_q only is not sufficient to guarantee the TSC for the nonextensive thermodynamics based on S_q^T . For $1 - q \geq 0$, however, the positivity of C_q guarantees to satisfy the Eq. (10) since $Z_q^{1-q} = \sum_i p_i^q$ is always positive. Note that the generalized temperature T_q is not equivalent to the physical temperature T , which is an intensive quantity and obeys the thermodynamic zeroth law. They are related by [13]

$$T = \{1 + (1 - q)S_q^T\} \cdot T_q. \quad (11)$$

By differentiating the both sides of Eq.(11) with respect to E , we obtain the relation between the specific heat $C \equiv \partial E / \partial T$ and the generalized specific heat C_q as

$$\frac{1}{C} = \frac{1 + (1 - q)S_q^T}{C_q} + 1 - q. \quad (12)$$

The TSC condition of Eq. (9) for S_q^T is thus equivalent to the positivity of the specific heat,

$$C \geq 0, \quad (13)$$

which is also equivalent to the conventional TSC.

Similar argument can be applied to the TSC for the normalized Tsallis entropy $S_{q,\text{no}}^T \equiv S_q^T / \sum_i p_i^q$ but one must take account of the fact that $S_{q,\text{no}}^T$ obeys the modified pseudo-additivity,

$$S_{q,\text{no}}^T(A, B) = S_{q,\text{no}}^T(A) + S_{q,\text{no}}^T(B) + (q - 1)S_{q,\text{no}}^T(A)S_{q,\text{no}}^T(B), \quad (14)$$

instead of the pseudo-additivity Eq. (2).

Now let us investigate the above results from the point of the view of the relation between Tsallis and Rényi entropies. Ramshaw [7] had obtained the same result of Eq. (5) by utilizing the relation Eq. (16) between the both entropies. Rényi entropy [12] is defined by,

$$S_q^R = \frac{\ln \sum_i p_i^q}{1 - q}, \quad (15)$$

which is additive for statistically independent systems, and a concave functions of the probabilities p_i for $0 < q < 1$. Indeed S_q^T and S_q^R are closely related by

$$S_q^R = \frac{\ln[1 + (1 - q)S_q^T]}{1 - q}. \quad (16)$$

For $1 - q > 0$, S_q^R is thus monotonically increasing function of S_q^T and vice versa. The extremization of either entropy subject to the same constraints will produce the same result. By differentiating twice the both sides of Eq. (16) with respect to E , we see that the concavity of $S_q^R(E)$, which is the TSC for $S_q^R(E)$, is equivalent to Eq. (6).

In order to further study the relation between the TSCs for the both entropies, we focus on the standard internal energy case (U), since there is no study based on Rényi entropy with the (un-)normalized q -average to the author's knowledge. Let us review the connection between the concavity (convexity) of an entropy \mathcal{S} with respect to the probability distributions $\mathbf{p} = (p_1, p_2, \dots)$ and the concavity (convexity) of \mathcal{S} with respect to the standard internal energy U . They are related by $\mathcal{S}(U) = \mathcal{S}(\mathbf{p}(U))$, where $\mathbf{p}(U)$ is the probability distribution obtained by extremizing $\mathcal{S}(\mathbf{p})$ subject to the constraint $U \equiv \sum_i p_i \epsilon_i$, and p_i is a probability of state i whose energy is ϵ_i . The result [7] is that the concavity (convexity) of $\mathcal{S}(\mathbf{p})$ implies the concavity (convexity) of $\mathcal{S}(U)$. The essence of the proof lies in the entropy extremum principle and no need to require the additivity of \mathcal{S} . The result thus holds for also non-additive Tsallis' entropy! Since $S_q^T(\mathbf{p})$ is concave for $q > 0$ [1,2], $S_q^T(U)$ is concave for $q > 0$. On the other hand Since $S_q^R(\mathbf{p})$ is concave for $0 < q < 1$ [12], $S_q^R(U)$ is concave for $0 < q < 1$.

Now let us consider what is deduced about the TSC for S_q^T from only the concavity of $S_q^T(U)$, which holds for $q > 0$. The concavity of $S_q^T(U)$ can be written by,

$$2S_q^T\left(\frac{U_a + U_b}{2}\right) \geq S_q^T(U_a) + S_q^T(U_b). \quad (17)$$

With the help of the arithmetic-geometric mean inequality ($\frac{a+b}{2} \geq \sqrt{ab}$ for

$a, b > 0$), we readily obtain

$$\frac{S_q^T(U_a) + S_q^T(U_b)}{2} \geq \sqrt{S_q^T(U_a)S_q^T(U_b)}, \quad (18)$$

since $S_q \geq 0$. Combining the Eqs. (17) and (18), we obtain

$$\left[S_q^T\left(\frac{U_a + U_b}{2}\right) \right]^2 \geq S_q^T(U_a)S_q^T(U_b). \quad (19)$$

Multiplying both sides of Eq. (19) by $(1 - q)$ and adding to both sides of Eq. (17), we obtain

$$\begin{aligned} 2S_q^T\left(\frac{U_a + U_b}{2}\right) + (1 - q) \left[S_q^T\left(\frac{U_a + U_b}{2}\right) \right]^2 \\ \geq S_q^T(U_a) + S_q^T(U_b) + (1 - q)S_q^T(U_a)S_q^T(U_b), \end{aligned} \quad (20)$$

if $1 - q \geq 0$, which is consistent with the condition that the functional relation of Eq. (16) guarantees the monotonic increase of S_q^R with S_q^T and vice versa. Since the concavity of $S_q^T(U)$ holds for $q > 0$, the resulting TSC of Eq. (20) is satisfied for $0 < q \leq 1$. Within the same range of q the TSC for S_q^R also holds since $S_q^R(U)$ is concave for $0 < q \leq 1$. The TSCs for the both entropies are therefore satisfied for $0 < q \leq 1$. This is consistent with the equivalence [7,13] between S_q^R and S_q^T for $0 < q \leq 1$.

In summary, the explicit differential form Eq. (6) of the TSC for S_q^T is derived by taking account of the pseudo-additivity of S_q^T . Unlike the TSC for conventional additive entropy, the concavity of $S_q^T(U)$ is not equivalent to the TSC for $S_q^T(U)$ due to the pseudo-additivity. The TSC for $S_q^T(U)$ is thus not simply related to the positivity of the generalized specific-heat C_q , which is equivalent to the concavity of $S_q^T(U)$, but related to the positivity of the specific heat C . These results are consistent with the relation between Tsallis and Rényi entropies for $0 < q \leq 1$. The author acknowledges Prof. S. Abe for useful comments and reading the manuscript.

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